PROJECT NUMBER: 2520
PROJECT TITLE: Flavor Research
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PERIOD COVERED: February, 1988

I. GLUCOSE-DERIVED FLAVORANTS

A. **Objective**: To develop glucose-derived flavorants.

B. **Results**: 1. Menthol-glucose carbonate. Since establishing that two compounds in the mixture of compounds known as menthol-glucose carbonate are particularly efficient at delivering menthol to mainstream smoke, efforts have been directed at enhancing their proportion in the mixture. Modification of reaction parameters did alter the product distribution in the desired direction. More recently, an alternate acylating agent has been investigated.

Reaction of glucose and 1-menthyloxycarbonylimidazolide in either pyridine or dimethylformamide in the presence of about 20 mol% of 1,8-diazabicyclo[5,4,0]undec-7-ene produced a reaction mixture which consisted of mainly 6-O, 2-O- and β-1-O-menthyloxycarbonyl-D-glucoses, with the 6-O-isomer being the more abundant one. However there is an extra component which corresponds to a monocarbonate. The identity of this component is under investigation.

2. Glucose-vanillin. Reaction of vanillin with acetobromoglucose in aqueous acetone produced 4'-formyl-2'-methoxyphenyl 2,3,4,6-tetra-O-acetyl-β-D-glucopyranoside in 57% yield. Subsequent hydrolysis with methanolic NaOH gave glucovanillin in 90% yield. Currently about 10 gm of glucovanillin is on hand.

II. PROJECT EXTRA

A. **Objective**: To develop proprietary flavor additives for enhanced flavor perception in low delivery cigarettes.

B. **Results**: 1. CR-2643 (6-methylhexahydro-2(H)-benzofuranone) has been shown to evince desirable subjective properties. A structurally similar tetrahydrobenzofuranone has been synthesized by a two-step reaction sequence in overall yield of 27%.

2. The synthesis of dihydroactinidiolide, a tobacco-identical benzofuranone, following a literature report gave a disappointing yield. Subsequent modification of conditions has revealed the reaction to be sensitive to the acidic conditions. A 60% yield of a mixture of the desired compound and another compound, aeginetolide, has been obtained thus far. Optimization of reaction conditions is being pursued.

3. The acylation of 2,3-dimethylpyrazine with isovaleraldehyde gave a 54% yield of the expected ketone (black pepper, slight chocolate aroma). This ketone was cleanly reduced with sodium

borohydride to give the corresponding alcohol (buttery, chocolate aroma). Several attempts to dehydrate this alcohol have been made; in most cases, the olefin was observed. However, the desired olefin is accompanied by varying amounts of disproportionation products.

4. Trimethylpyrazine was acylated with isovaleraldehyde to give the ketone in 67% yield. A portion of the ketone was converted to the hydrazone for subsequent reduction to the alkylpyrazine.